

FILE 'HOME' ENTERED AT 12:32:06 ON 03 JUN 2003

=> file reg

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

0.21

0.21

FILE 'REGISTRY' ENTERED AT 12:32:15 ON 03 JUN 2003

USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.

PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 1 JUN 2003 HIGHEST RN 523977-56-2

DICTIONARY FILE UPDATES: 1 JUN 2003 HIGHEST RN 523977-56-2

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2003

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. See HELP PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry File, for complete details:

<http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf>

=>

Uploading 09975136 before allowance.str

L1 STRUCTURE UPLOADED

=> id l1

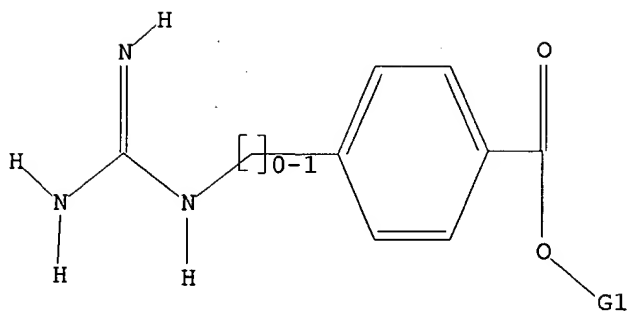
COMBINATION OF STRUCTURE AND TEXT TERMS NOT VALID

The query entered contains both search terms created by structure-building or screen commands and text search terms. L#s created via the STRUCTURE or SCREEN commands must be searched in the structures files separately from text terms or profiles. The L# answer sets from structure searches can be used in crossover searches and can be combined with text terms.

=> d l1

L1 HAS NO ANSWERS

L1 STR



G1 H,Cb,Ak

Structure attributes must be viewed using STN Express query preparation.

=> search l1 sss sam

SAMPLE SEARCH INITIATED 12:32:49 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 208 TO ITERATE

100.0% PROCESSED 208 ITERATIONS

50 ANSWERS

INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 3295 TO 5025

PROJECTED ANSWERS: 1047 TO 2113

L2 50 SEA SSS SAM L1

=> d scan

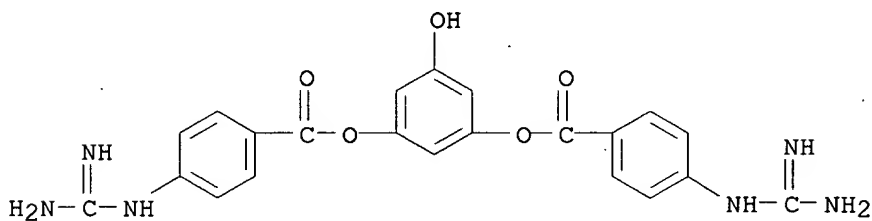
L2 50 ANSWERS REGISTRY COPYRIGHT 2003 ACS

IN Benzoic acid, 4-[(aminoiminomethyl)amino]-, 5-hydroxy-1,3-phenylene ester,

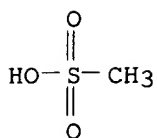
dimethanesulfonate (salt) (9CI)

MF C22 H20 N6 O5 . 2 C H4 O3 S

CM 1

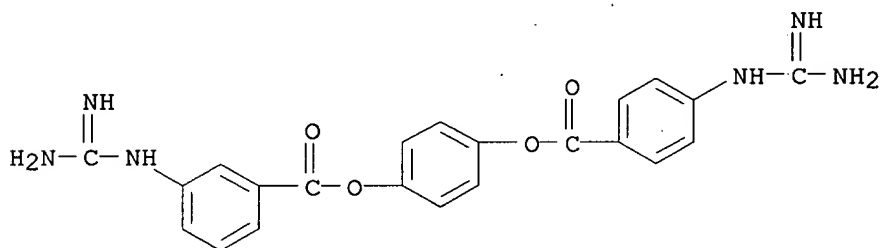


CM 2



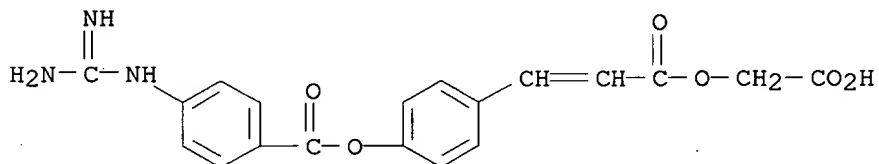
HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):5

L2 50 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN Benzoic acid, 3-[(aminoiminomethyl)amino]-, 4-[[4-
 [(aminoiminomethyl)amino]benzoyl]oxy]phenyl ester (9CI)
 MF C22 H20 N6 O4



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 50 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN Benzoic acid, 4-[(aminoiminomethyl)amino]-,
 4-[3-(carboxymethoxy)-3-oxo-1-
 propenyl]phenyl ester (9CI)
 MF C19 H17 N3 O6
 CI COM



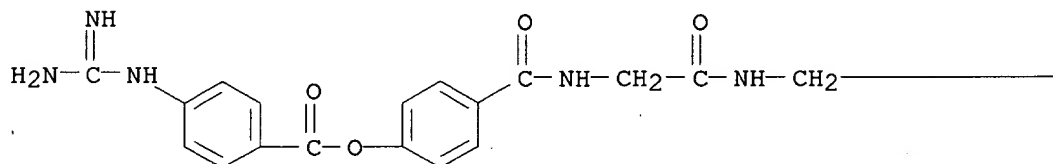
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 50 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN Poly(oxy-1,2-ethanediyl), .alpha.-[2-[[[4-[[4-

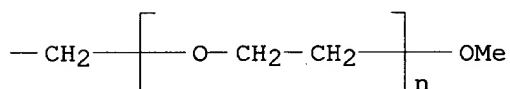
[(aminoiminomethyl)amino]benzoyl]oxy]benzoyl]amino]acetyl]amino]ethyl}-
 .omega.-methoxy-, monomethanesulfonate (9CI)
 MF (C2 H4 O)n C20 H23 N5 O5 . C H4 O3 S

CM 1

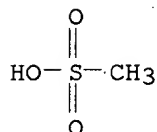
PAGE 1-A



PAGE 1-B

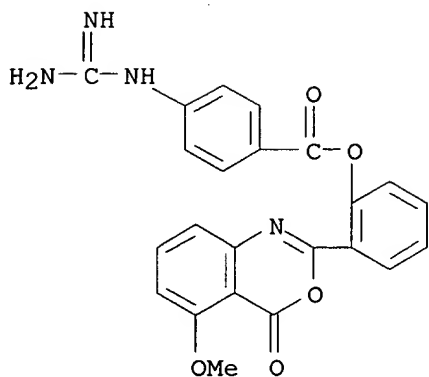


CM 2

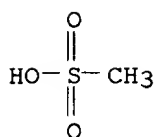


L2 50 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN Benzoic acid, 4-[(aminoiminomethyl)amino]-, 2-(5-methoxy-4-oxo-4H-3,1-
 benzoxazin-2-yl)phenyl ester, monomethanesulfonate (9CI)
 MF C23 H18 N4 O5 . C H4 O3 S

CM 1

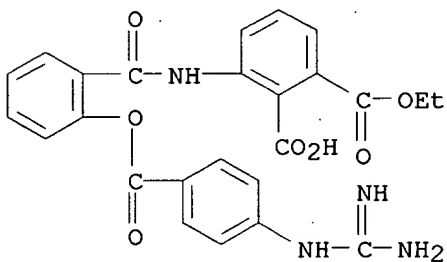


CM 2

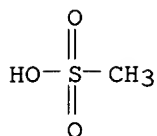


L2 50 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN 1,2-Benzenedicarboxylic acid,
 3-[[2-[[4-[(aminoiminomethyl)amino]benzoyl]oxy]benzoyl]amino]-, 1-ethyl ester, monomethanesulfonate (9CI)
 MF C25 H22 N4 O7 . C H4 O3 S

CM 1



CM 2



HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):30

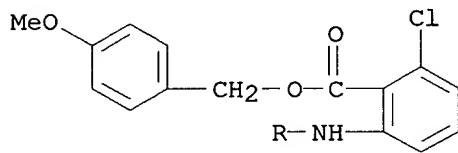
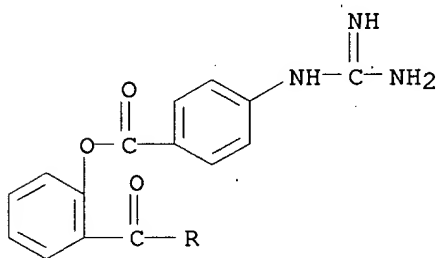
L2 50 ANSWERS REGISTRY COPYRIGHT 2003 ACS

IN Benzoic acid,

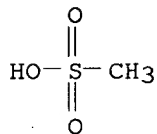
2-[[2-[[4-[(aminoiminomethyl)amino]benzoyl]oxy]benzoyl]amino
]-6-chloro-, (4-methoxyphenyl)methyl ester, monomethanesulfonate (9CI)

MF C30 H25 Cl N4 O6 . C H4 O3 S

CM 1



CM 2

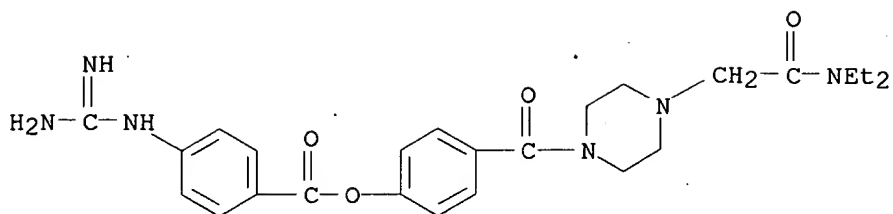


L2 50 ANSWERS REGISTRY COPYRIGHT 2003 ACS

IN Benzoic acid, 4-[(aminoiminomethyl)amino]-, 4-[[4-[2-(diethylamino)-2-oxoethyl]-1-piperazinyl]carbonyl]phenyl ester (9CI)

MF C25 H32 N6 O4

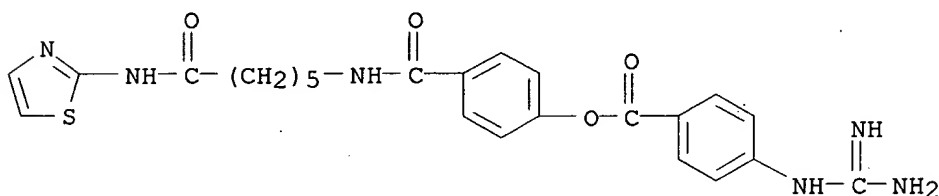
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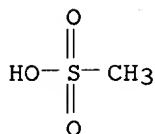
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 50 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN Benzoic acid, 4-[(aminoiminomethyl)amino]-, 4-[[[6-oxo-6-(2-thiazolylamino)hexyl]amino]carbonyl]phenyl ester, monomethanesulfonate (9CI)
 MF C24 H26 N6 O4 S . C H4 O3 S

CM 1

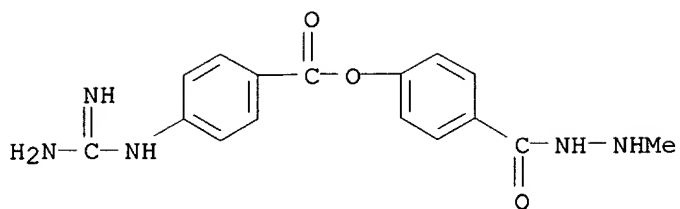


CM 2

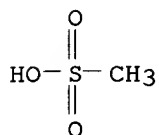


L2 50 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN Benzoic acid, 4-[(aminoiminomethyl)amino]-, 4-[(2-methylhydrazino)carbonyl]phenyl ester, monomethanesulfonate (9CI)
 MF C16 H17 N5 O3 . C H4 O3 S

CM 1

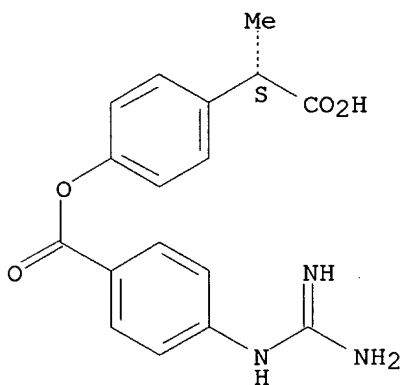


CM 2



L2 50 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN Benzeneacetic acid, 4-[[4-[(aminoiminomethyl)amino]benzoyl]oxy]-.alpha.-
 methyl-, (S)- (9CI)
 MF C17 H17 N3 O4
 CI COM

Absolute stereochemistry.

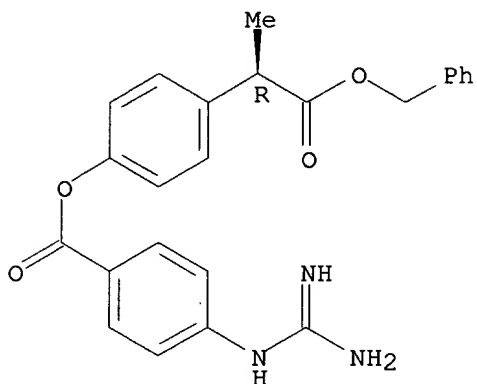


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

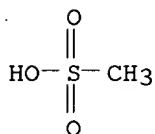
L2 50 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN Benzeneacetic acid, 4-[[4-[(aminoiminomethyl)amino]benzoyl]oxy]-.alpha.-
 methyl-, phenylmethyl ester, (R)-, monomethanesulfonate (9CI)
 MF C24 H23 N3 O4 . C H4 O3 S

CM 1

Absolute stereochemistry.

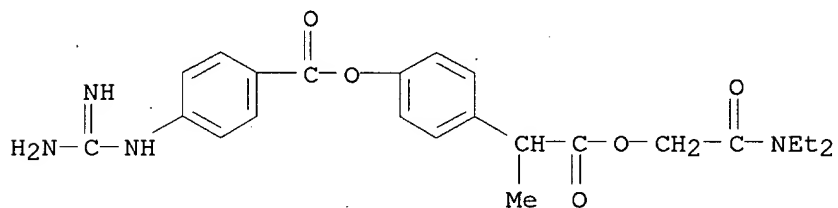


CM 2

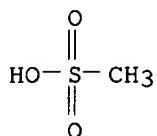


L2 50 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Benzeneacetic acid, 4-[[4-[(aminoiminomethyl)amino]benzoyl]oxy]-.alpha.-methyl-, 2-(diethylamino)-2-oxoethyl ester, monomethanesulfonate (9CI)
MF C23 H28 N4 O5 . C H4 O3 S

CM 1

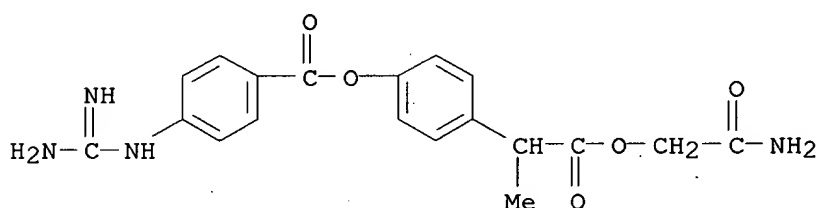


CM 2

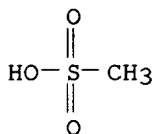


L2 50 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN Benzeneacetic acid, 4-[[4-[(aminoiminomethyl)amino]benzoyl]oxy]-.alpha.-methyl-, 2-amino-2-oxoethyl ester, monomethanesulfonate (9CI)
 MF C19 H20 N4 O5 . C H4 O3 S

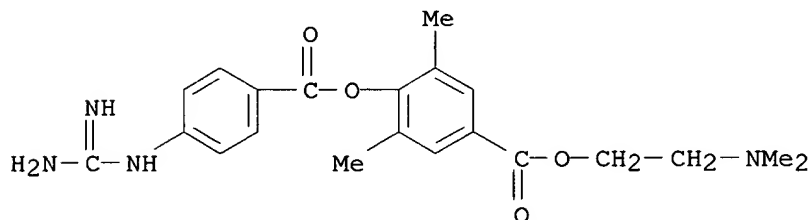
CM 1



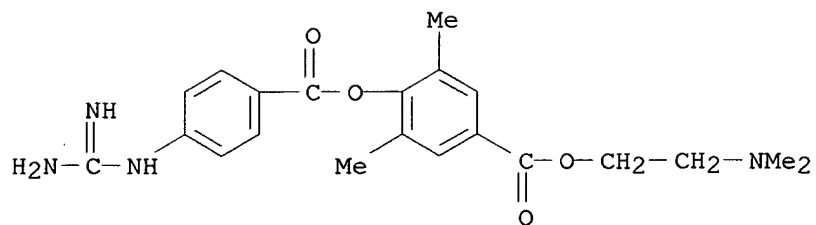
CM 2



L2 50 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN Benzoic acid, 4-[[4-[(aminoiminomethyl)amino]benzoyl]oxy]-3,5-dimethyl-, 2-(dimethylamino)ethyl ester, dihydrochloride (9CI)
 MF C21 H26 N4 O4 . 2 Cl H



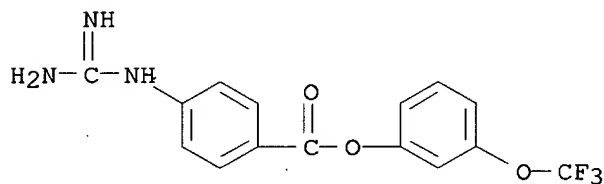
● 2 HCl



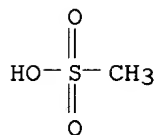
● 2 HCl

L2 50 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN Benzoic acid, 4-[(aminoiminomethyl)amino]-, 3-(trifluoromethoxy)phenyl
 ester, monomethanesulfonate (9CI)
 MF C15 H12 F3 N3 O3 . C H4 O3 S

CM 1

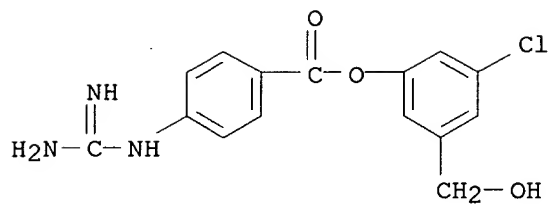


CM 2

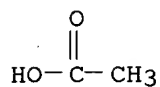


L2 50 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN Benzoic acid, 4-[(aminoiminomethyl)amino]-, 3-chloro-5-
 (hydroxymethyl)phenyl ester, monoacetate (salt) (9CI)
 MF C15 H14 Cl N3 O3 . C2 H4 O2

CM 1

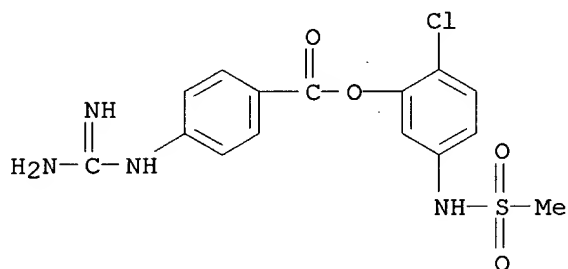


CM 2

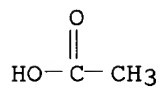


L2 50 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN Benzoic acid, 4-[(aminoiminomethyl)amino]-, 2-chloro-5-
 [(methylsulfonyl)amino]phenyl ester, monoacetate (9CI)
 MF C15 H15 Cl N4 O4 S . C2 H4 O2

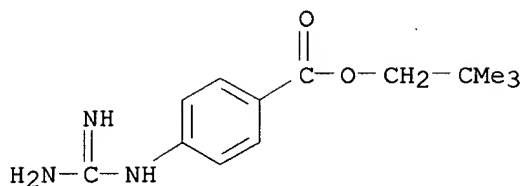
CM 1



CM 2



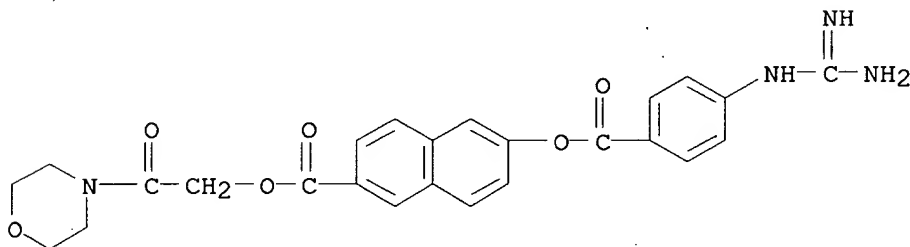
L2 50 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN Benzoic acid, 4-[(aminoiminomethyl)amino]-, 2,2-dimethylpropyl ester
 (9CI)
 MF C13 H19 N3 O2



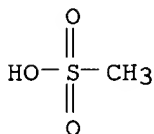
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 50 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN 2-Naphthalenecarboxylic acid,
 6-[[4-[(aminoiminomethyl)amino]benzoyl]oxy]-
 , 2-(4-morpholinyl)-2-oxoethyl ester, monomethanesulfonate (9CI)
 MF C25 H24 N4 O6 . C H4 O3 S

CM 1

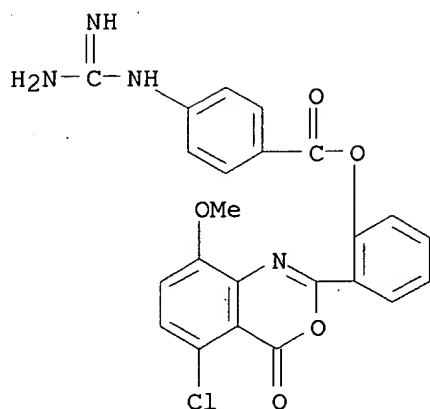


CM 2

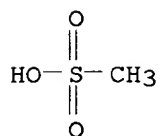


L2 50 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN Benzoic acid, 4-[(aminoiminomethyl)amino]-,
 2-(5-chloro-8-methoxy-4-oxo-4H-
 3,1-benzoxazin-2-yl)phenyl ester, monomethanesulfonate (9CI)
 MF C23 H17 Cl N4 O5 . C H4 O3 S

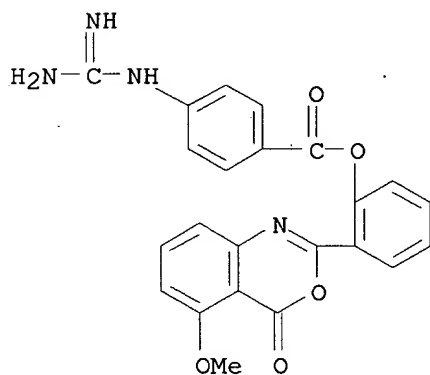
CM 1



CM 2

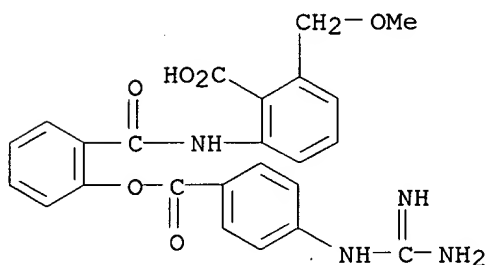


L2 50 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN Benzoic acid, 4-[(aminoiminomethyl)amino]-, 2-(5-methoxy-4-oxo-4H-3,1-benzoxazin-2-yl)phenyl ester (9CI)
 MF C23 H18 N4 O5
 CI COM



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

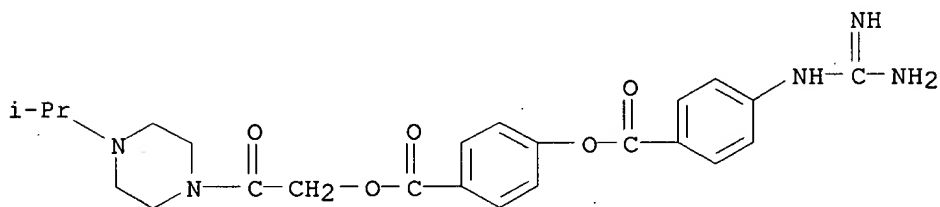
L2 50 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN Benzoic acid,
 2-[[2-[[4-[(aminoiminomethyl)amino]benzoyl]oxy]benzoyl]amino
]-6-(methoxymethyl)- (9CI)
 MF C24 H22 N4 O6
 CI COM



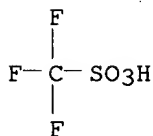
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 50 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN Benzoic acid, 4-[(aminoiminomethyl)amino]-, 4-[[2-[4-(1-methylethyl)-1-piperazinyl]-2-oxoethoxy]carbonyl]phenyl ester,
 mono(trifluoromethanesulfonate) (9CI)
 MF C24 H29 N5 O5 . C H F3 O3 S

CM 1

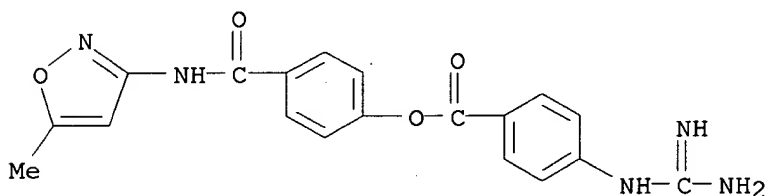


CM 2

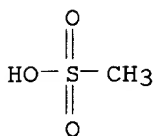


L2 50 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN Benzoic acid, 4-[(aminoiminomethyl)amino]-, 4-[[5-methyl-3-isoxazolyl)amino]carbonyl]phenyl ester, monomethanesulfonate (9CI)
 MF C19 H17 N5 O4 . C H4 O3 S

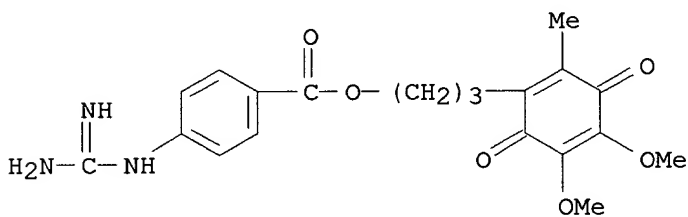
CM 1



CM 2



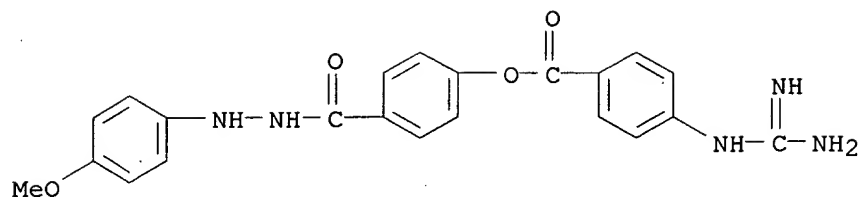
L2 50 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN Benzoic acid, 4-[(aminoiminomethyl)amino]-, 3-(4,5-dimethoxy-2-methyl-3,6-dioxo-1,4-cyclohexadien-1-yl)propyl ester (9CI)
 MF C20 H23 N3 O6



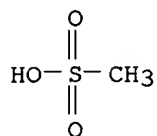
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 50 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN Benzoic acid, 4-[(aminoiminomethyl)amino]-, 4-[[2-(4-methoxyphenyl)hydrazino]carbonyl]phenyl ester, monomethanesulfonate (9CI)
 MF C22 H21 N5 O4 . C H4 O3 S

CM 1

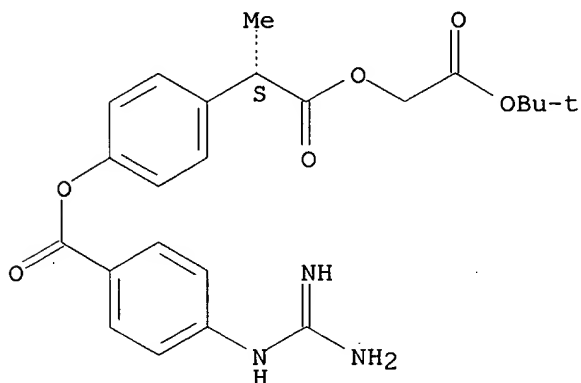


CM 2



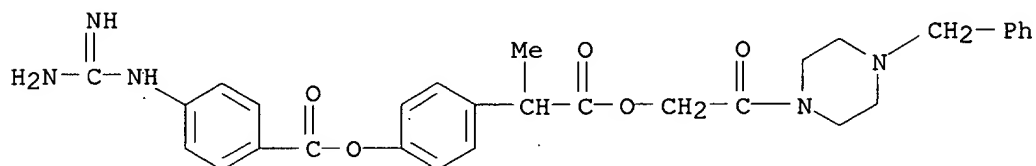
L2 50 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Benzeneacetic acid, 4-[[4-[(aminomethyl)amino]benzoyl]oxy]-.alpha.-
methyl-, 2-(1,1-dimethylethoxy)-2-oxoethyl ester, (S)- (9CI)
MF C23 H27 N3 O6
CI COM

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

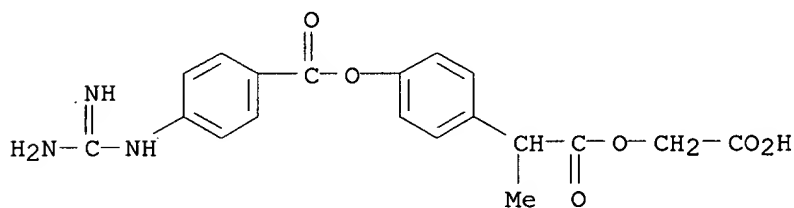
L2 50 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN Benzeneacetic acid, 4-[[4-[(aminoiminomethyl)amino]benzoyl]oxy]-.alpha.-methyl-, 2-oxo-2-[4-(phenylmethyl)-1-piperazinyl]ethyl ester (9CI)
 MF C30 H33 N5 O5
 CI COM



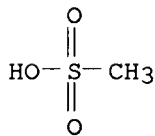
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 50 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN Benzeneacetic acid, 4-[[4-[(aminoiminomethyl)amino]benzoyl]oxy]-.alpha.-methyl-, carboxymethyl ester, monomethanesulfonate (9CI)
 MF C19 H19 N3 O6 . C H4 O3 S

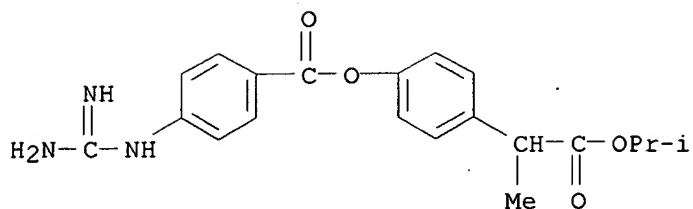
CM 1



CM 2

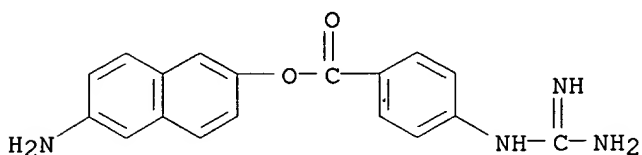


L2 50 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN Benzeneacetic acid, 4-[[4-[(aminoiminomethyl)amino]benzoyl]oxy]-.alpha.-methyl-, 1-methylethyl ester (9CI)
 MF C20 H23 N3 O4
 CI COM

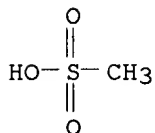


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

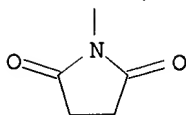
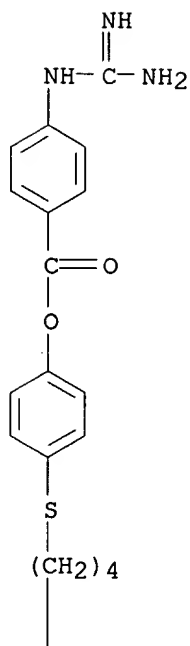
L2 50 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN Benzoic acid, 4-[(aminoiminomethyl)amino]-, 6-amino-2-naphthalenyl ester,
 dimethanesulfonate (9CI)
 MF C18 H16 N4 O2 . 2 C H4 O3 S
 CM 1



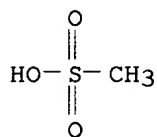
CM 2



L2 50 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN Benzoic acid, 4-[(aminoiminomethyl)amino]-, 4-[[4-(2,5-dioxo-1-
 pyrrolidinyl)butyl]thio]phenyl ester, monomethanesulfonate (9CI)
 MF C22 H24 N4 O4 S . C H4 O3 S
 CM 1



CM 2

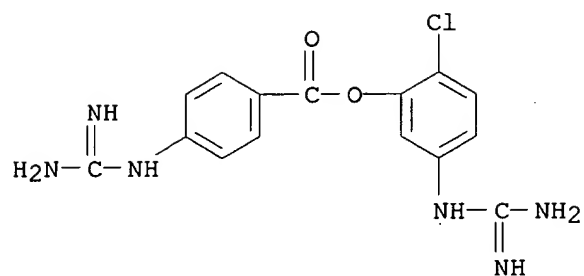


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

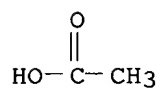
L2 50 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN Benzoic acid, 4-[(aminoiminomethyl)amino]-,
 5-[(aminoiminomethyl)amino]-2-
 chlorophenyl ester, diacetate (9CI)

MF C15 H15 Cl N6 O2 . 2 C2 H4 O2

CM 1

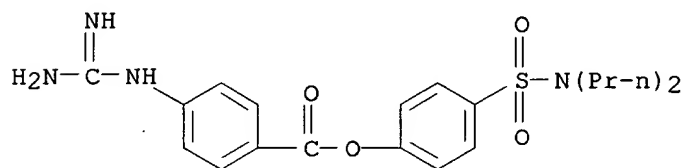


CM 2

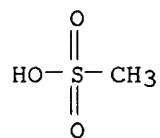


L2 50 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Benzoic acid, 4-[(aminoiminomethyl)amino]-, 4-
[(dipropylamino)sulfonyl]phenyl ester, monomethanesulfonate (9CI)
MF C20 H26 N4 O4 S . C H4 O3 S

CM 1

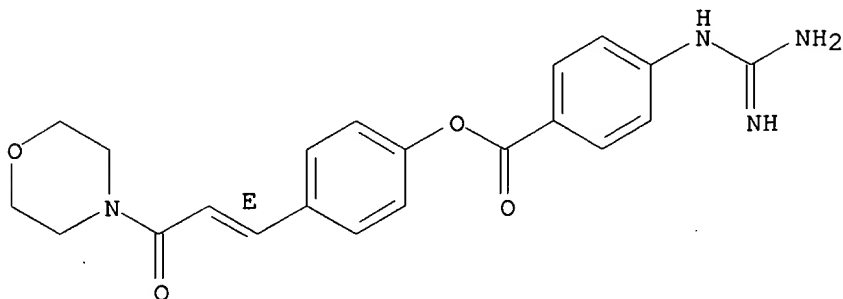


CM 2



L2 50 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Benzoic acid, 4-[(aminoiminomethyl)amino]-, 4-[(1E)-3-(4-morpholinyl)-3-oxo-1-propenyl]phenyl ester (9CI)
MF C21 H22 N4 O4
CI COM

Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):o
'O' IS NOT VALID HERE

To display more answers, enter the number of answers you would like to see. To end the display, enter "NONE", "N", "0", or "END".

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

=> search l1 sss full

FULL SEARCH INITIATED 12:34:48 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 3885 TO ITERATE

100.0% PROCESSED 3885 ITERATIONS
SEARCH TIME: 00.00.01

1258 ANSWERS

L3 1258 SEA SSS FUL L1

=> file caplus

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

149.75

149.96

FILE 'CAPLUS' ENTERED AT 12:34:57 ON 03 JUN 2003

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FILE COVERS 1907 - 3 Jun 2003 VOL 138 ISS 23
FILE LAST UPDATED: 2 Jun 2003 (20030602/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> 13

L4 876 L3

=> ?bact?

L5 613320 ?BACT?

=> 14 and 15

L6 31 L4 AND L5

=> d 16 20-31 ti

L6 ANSWER 20 OF 31 CAPLUS COPYRIGHT 2003 ACS
TI Probiotics: antistaphylococcal activity of 4-aminocyclohexanecarboxylic acid, aminobenzoic acid, and their derivatives and structure-activity relations

L6 ANSWER 21 OF 31 CAPLUS COPYRIGHT 2003 ACS
TI Cephalosporin compounds

L6 ANSWER 22 OF 31 CAPLUS COPYRIGHT 2003 ACS
TI The protease inhibitor p-nitrophenyl-p'-guanidinobenzoate inactivates Sindbis and other enveloped viruses

L6 ANSWER 23 OF 31 CAPLUS COPYRIGHT 2003 ACS
TI 6-[.alpha.-(.omega.-Guanidinoalkanoylamido)acylamido]penicillanic acids

L6 ANSWER 24 OF 31 CAPLUS COPYRIGHT 2003 ACS
TI 6-[.alpha.-(.omega.-Guanidinoalkanoylamido)acylamido]penicillanic acids

L6 ANSWER 25 OF 31 CAPLUS COPYRIGHT 2003 ACS
TI Influence of various proteinase inhibitors on the gelatinolytic effect of ejaculated and uterine boar spermatozoa

L6 ANSWER 26 OF 31 CAPLUS COPYRIGHT 2003 ACS
TI Pharmaceutical cephalosporins

L6 ANSWER 27 OF 31 CAPLUS COPYRIGHT 2003 ACS
TI Antimicrobial and hypoglycemic (2-imidazolidinylidene)- and (hexahydro-2-pyrimidinylidene)guanidines

L6 ANSWER 28 OF 31 CAPLUS COPYRIGHT 2003 ACS
TI Specificity and mechanism of clostripain catalysis

L6 ANSWER 29 OF 31 CAPLUS COPYRIGHT 2003 ACS
TI **Antibacterial** guanidinoarylpenicillins

L6 ANSWER 30 OF 31 CAPLUS COPYRIGHT 2003 ACS
 TI Tuberculostatic activity of derivatives of aminoguanidine and
 diaminoguanidine and its correlation with chemical structure

L6 ANSWER 31 OF 31 CAPLUS COPYRIGHT 2003 ACS
 TI Reaction of cyanoguanidine with aromatic amines. II. Formation of
 1-amidino-3-(p-nitrophenyl- and p-carboxyphenyl)urea

=> pylori

7936 PYLORI
 20 PYLORIS
 L7 7949 PYLORI
 (PYLORI OR PYLORIS)

=> l4 and l7

L8 2 L4 AND L7

=> d l8 1-2 ti

L8 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2003 ACS
 TI Preparation of esters of 4-guanidiny(methyl)benzoic acid treating or
 preventing bacterial infection

L8 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2003 ACS
 TI Enzyme inhibitors for treatment of gastrointestinal disorders caused by
 Helicobacter pylori

=> d l8 1-2 ti fbib abs

L8 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2003 ACS
 TI Preparation of esters of 4-guanidiny(methyl)benzoic acid treating or
 preventing bacterial infection
 AN 2003:282526 CAPLUS
 DN 138:304065
 TI Preparation of esters of 4-guanidiny(methyl)benzoic acid treating or
 preventing bacterial infection
 IN Zhu, Dexu; Muramatsu, Mutsumi; Xie, Jianshu; Cheng, Ni; Wang, Mingwei
 PA Peop. Rep. China
 SO PCT Int. Appl., 43 pp.
 CODEN: PIXXD2
 DT Patent
 LA English
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2003029201	A1	20030410	WO 2001-CN1499	20011023
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,				
	CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,				
	GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,				
	LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL,				
	PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG,				
	US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY,				
	DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF,				
	BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				

GI



0.10

RE.CNT 2

L8 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2003 ACS

AN 1994:587325 CAPLUS

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	DE 4305536	A1	19940825	DE 1993-4305536	19930219
	WO 9418964	A1	19940901	WO 1994-EP523	19940218
	W: AU, CA, FI, HU, JP, NO, US				
	RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
	AU 9462053	A1	19940914	DE 1993-4305536A	19930219
				AU 1994-62053	19940218
				DE 1993-4305536A	19930219
				WO 1994-EP523 W	19940218
	EP 804184	A1	19971105	EP 1994-909036	19940218
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE				
				DE 1993-4305536A	19930219
				WO 1994-EP523 W	19940218
	JP 2002515002	T2	20020521	JP 1994-518670	19940218
				DE 1993-4305536A	19930219
			WO 1994-EP523 W	19940218	
	WO 9614068	A1	19960517	WO 1994-EP3669	19941107

W: AT, CA, FI, HU, JP, NO, US

RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE
DE 1993-4305536 19930219

AB Enzyme inhibitors, esp. protease inhibitors such as .omega.-
guanidinocarboxylic acid esters, are useful for treatment of H.
pylori-assocd. gastrointestinal disorders. Thus, soft gelatin
capsules contained camostat 100.00, soybean lecithin 5.00,
2,6-di-tert-butyl-4-methylphenol (antioxidant) 0.1, and peanut oil to
800.00 mg.

=> d 18 2 it

L8 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2003 ACS

IT Carboxylic acids, biological studies

RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(guanidino, esters, Helicobacter **pylori**-assocd. digestive
disorder treatment with)

IT Campylobacter pyloridis

(infection with, digestive disorder from, treatment of, with
proteinase
inhibitors)

IT Enzymes

RL: BSU (Biological study, unclassified); BIOL (Biological study)
(inhibitors, Helicobacter **pylori**-assocd. digestive disorder
treatment with)

IT Digestive tract

(disease, infection, with Helicobacter **pylori**, treatment of,
with proteinase inhibitors)

IT Onium compounds

RL: BIOL (Biological study)
(guanidinium, carboxy, Helicobacter **pylori**-assocd. digestive
disorder treatment with)

IT 6659-35-4D, .epsilon.-Guanidinocaproic acid, esters **16060-65-4D**,
p-Guanidinobenzoic acid, esters 37205-61-1, Proteinase inhibitor
39492-01-8, Gabexate **59721-28-7**, Camostat **71079-09-9**,
FOY 251 **81525-10-2**, Nafamostat

RL: BIOL (Biological study)
(Helicobacter **pylori**-assocd. digestive disorder treatment
with)

=> 59721-28-7

REGISTRY INITIATED

Substance data SEARCH and crossover from CAS REGISTRY in progress...
Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

L10

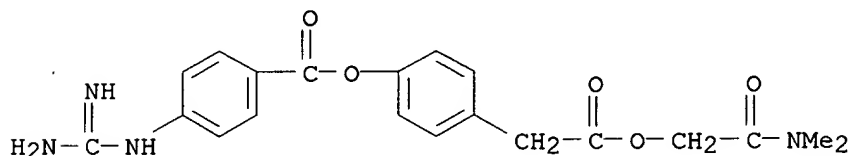
82 L9

=> display hitstr

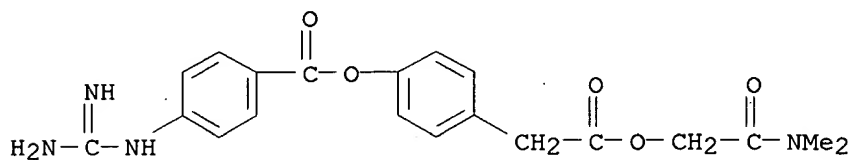
ENTER (L10), L# OR ?:110

ENTER ANSWER NUMBER OR RANGE (1):1-5

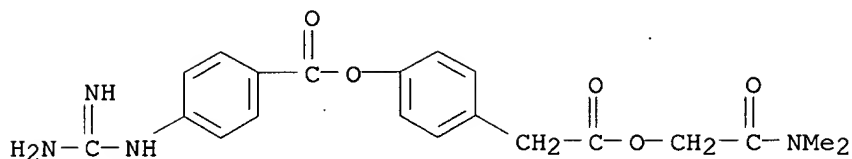
L10 ANSWER 1 OF 82 CAPLUS COPYRIGHT 2003 ACS
 IT **59721-28-7**, Camostat
 RL: BSU (Biological study, unclassified); BIOL (Biological study)
 (development of camostat mesilate troche for prevention of mucositis
 in
 mouth during cancer chemotherapy (Erratum))
 RN 59721-28-7 CAPLUS
 CN Benzeneacetic acid, 4-[[4-[(aminoiminomethyl)amino]benzoyl]oxy]-,
 2-(dimethylamino)-2-oxoethyl ester (9CI) (CA INDEX NAME)



L10 ANSWER 2 OF 82 CAPLUS COPYRIGHT 2003 ACS
 IT **59721-28-7**, Camostat
 RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
 (Biological study); USES (Uses)
 (trypsin inhibitor camostat has different effects on pancreas between
 cholecystokinin-A receptor gene knockout and wild-type mice)
 RN 59721-28-7 CAPLUS
 CN Benzeneacetic acid, 4-[[4-[(aminoiminomethyl)amino]benzoyl]oxy]-,
 2-(dimethylamino)-2-oxoethyl ester (9CI) (CA INDEX NAME)



L10 ANSWER 3 OF 82 CAPLUS COPYRIGHT 2003 ACS
 IT **59721-28-7**, Camostat
 RL: BSU (Biological study, unclassified); BIOL (Biological study)
 (metabolite; development of camostat mesilate troche for prevention of
 mucositis in mouth during cancer chemotherapy)
 RN 59721-28-7 CAPLUS
 CN Benzeneacetic acid, 4-[[4-[(aminoiminomethyl)amino]benzoyl]oxy]-,
 2-(dimethylamino)-2-oxoethyl ester (9CI) (CA INDEX NAME)



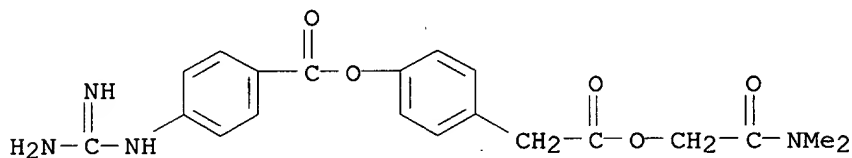
L10 ANSWER 4 OF 82 CAPLUS COPYRIGHT 2003 ACS

IT 59721-28-7

RL: FFD (Food or feed use); BIOL (Biological study); USES (Uses)
(fish feed contg. proteinase inhibitors)

RN 59721-28-7 CAPLUS

CN Benzeneacetic acid, 4-[[4-[(aminoiminomethyl)amino]benzoyl]oxy]-,
2-(dimethylamino)-2-oxoethyl ester (9CI) (CA INDEX NAME)



L10 ANSWER 5 OF 82 CAPLUS COPYRIGHT 2003 ACS

IT 59721-28-7, Camostat

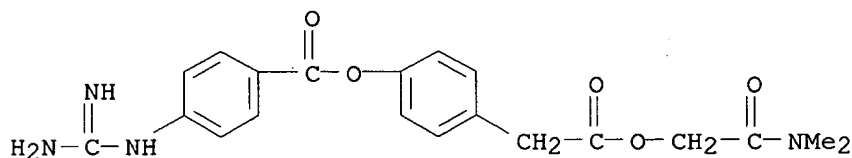
RL: PEP (Physical, engineering or chemical process); PRP (Properties);

THU

(Therapeutic use); BIOL (Biological study); PROC (Process); USES (Uses)
(prepn. and characterization of biodegradable or enteric-coated
microspheres contg. the protease inhibitor camostat)

RN 59721-28-7 CAPLUS

CN Benzeneacetic acid, 4-[[4-[(aminoiminomethyl)amino]benzoyl]oxy]-,
2-(dimethylamino)-2-oxoethyl ester (9CI) (CA INDEX NAME)



=> logoff hold

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

13.16

179.28

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE

TOTAL

CA SUBSCRIBER PRICE	ENTRY	SESSION
	0.00	-1.30

SESSION WILL BE HELD FOR 60 MINUTES
STN INTERNATIONAL SESSION SUSPENDED AT 12:40:34 ON 03 JUN 2003

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:sssptal623paz

PASSWORD:

* * * * * RECONNECTED TO STN INTERNATIONAL * * * * *
SESSION RESUMED IN FILE 'CAPLUS' AT 12:42:25 ON 03 JUN 2003
FILE 'CAPLUS' ENTERED AT 12:42:25 ON 03 JUN 2003
COPYRIGHT (C) 2003 AMERICAN CHEMICAL SOCIETY (ACS)

COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	13.16	179.28

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	0.00	-1.30

=> file reg

COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	13.58	179.70

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	0.00	-1.30

FILE 'REGISTRY' ENTERED AT 12:42:50 ON 03 JUN 2003
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
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Property values tagged with IC are from the ZIC/VINITI data file
provided by InfoChem.

STRUCTURE FILE UPDATES: 1 JUN 2003 HIGHEST RN 523977-56-2
DICTIONARY FILE UPDATES: 1 JUN 2003 HIGHEST RN 523977-56-2

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2003

Please note that search-term pricing does apply when
conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. See HELP
PROPERTIES for more information. See STNnote 27, Searching Properties

in the CAS Registry File, for complete details:
<http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf>

=>

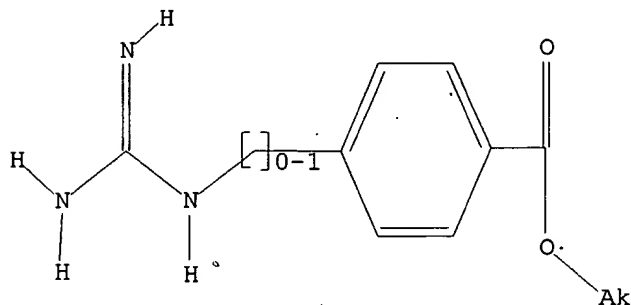
Uploading 09975136 before allowance.str

L11 STRUCTURE UPLOADED

=> d l11

L11 HAS NO ANSWERS

L11 STR



G1 H,Cb,Ak

Structure attributes must be viewed using STN Express query preparation.

=> search l11 sss sam

SAMPLE SEARCH INITIATED 12:43:23 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 208 TO ITERATE

100.0% PROCESSED 208 ITERATIONS

9 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 3295 TO 5025

PROJECTED ANSWERS: 9 TO 360

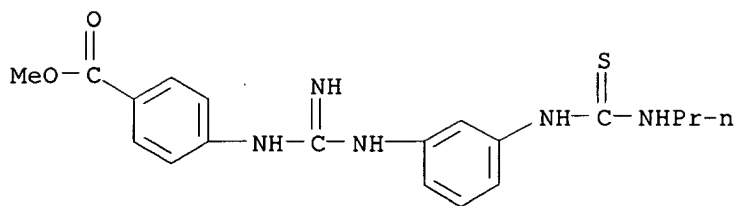
L12 9 SEA SSS SAM L11

=> d scan

L12 9 ANSWERS REGISTRY COPYRIGHT 2003 ACS

IN Benzoic acid, p-[3-[m-(3-propyl-2-thioureido)phenyl]guanidino]-, methyl
 ester, monohydrochloride (8CI)

MF C19 H23 N5 O2 S . Cl H



● HCl

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

=>

=>

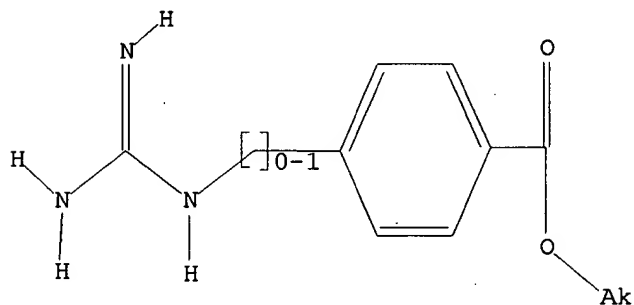
Uploading 09975136 before allowance.str

L13 STRUCTURE UPLOADED

=> d 113

L13 HAS NO ANSWERS

L13 STR



G1 H, Ob, Ak

Structure attributes must be viewed using STN Express query preparation.

=> search 113 sss sam

SAMPLE SEARCH INITIATED 12:45:00 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 208 TO ITERATE

100.0% PROCESSED 208 ITERATIONS

9 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 3295 TO 5025

PROJECTED ANSWERS: 9 TO 360

L14

9 SEA SSS SAM L13

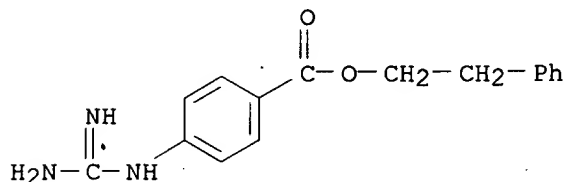
=> d scan

L14 9 ANSWERS REGISTRY COPYRIGHT 2003 ACS

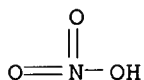
IN Benzoic acid, 4-[(aminoiminomethyl)amino]-, 2-phenylethyl ester, mononitrate (9CI)

MF C16 H17 N3 O2 . H N O3

CM 1



CM 2



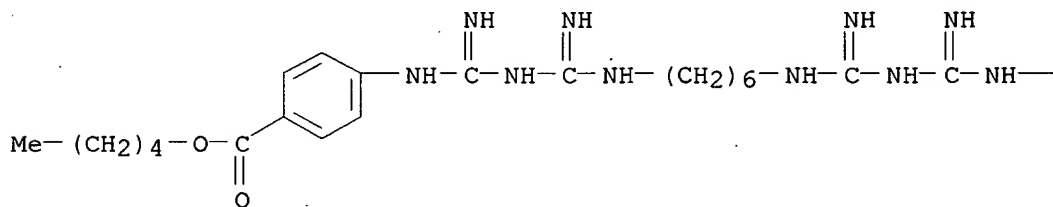
HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):8

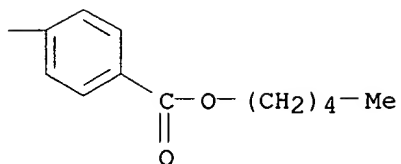
L14 9 ANSWERS REGISTRY COPYRIGHT 2003 ACS

IN Benzoic acid, 4,4'-[(1,3,12,14-tetraimino-2,4,11,13-tetraazatetradecane-1,14-diyl)diimino]bis-, dipentyl ester, dihydrochloride (9CI)

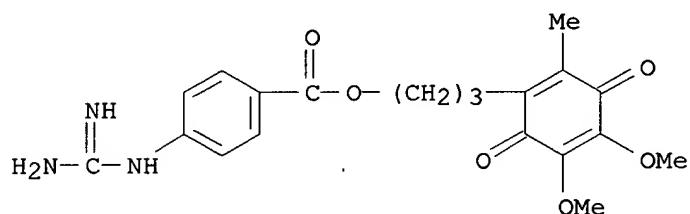
MF C34 H52 N10 O4 . 2 Cl H

PAGE 1-A



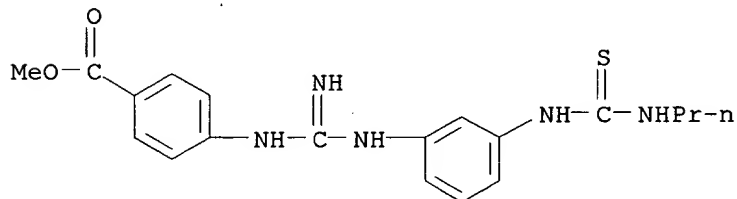


L14 9 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN Benzoic acid, 4-[(aminoiminomethyl)amino]-,
 3-(4,5-dimethoxy-2-methyl-3,6-
 dioxo-1,4-cyclohexadien-1-yl)propyl ester (9CI)
 MF C20 H23 N3 O6



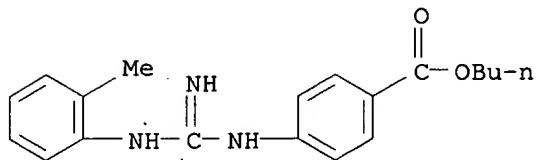
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L14 9 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN Benzoic acid, p-[3-[m-(3-propyl-2-thioureido)phenyl]guanidino]-, methyl
 ester, monohydrochloride (8CI)
 MF C19 H23 N5 O2 S . Cl H



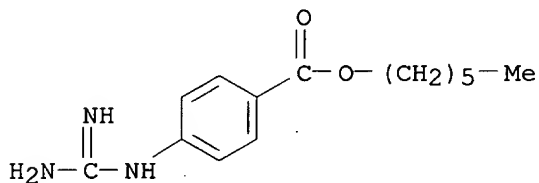
● HCl

L14 9 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN Benzoic acid, 4-[[imino[(2-methylphenyl)amino]methyl]amino]-, butyl ester
 (9CI)
 MF C19 H23 N3 O2



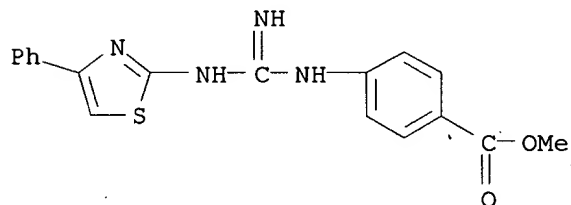
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L14 9 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN Benzoic acid, 4-[(aminoiminomethyl)amino]-, hexyl ester (9CI)
 MF C14 H21 N3 O2
 CI COM



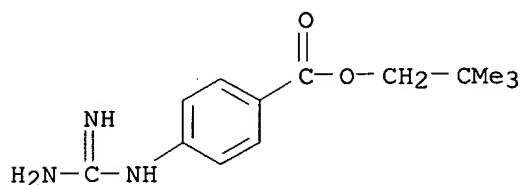
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L14 9 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN Benzoic acid, 4-[[imino[(4-phenyl-2-thiazolyl)amino]methyl]amino]-,
 methyl
 ester (9CI)
 MF C18 H16 N4 O2 S



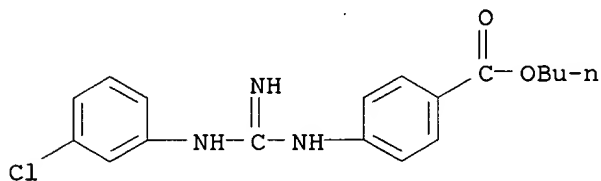
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L14 9 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Benzoic acid, 4-[(aminoiminomethyl)amino]-, 2,2-dimethylpropyl ester
(9CI)
MF C13 H19 N3 O2



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L14 9 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Benzoic acid, 4-[[[(3-chlorophenyl)amino]iminomethyl]amino]-, butyl ester
(9CI).
MF C18 H20 Cl N3 O2



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

ALL ANSWERS HAVE BEEN SCANNED

=> e Benzoic acid, 4-[(aminoiminomethyl)amino]-, 2,2-dimethylpropyl ester/cn
E1 1 BENZOIC ACID,
4,6-DIMETHOXY-3-(5-METHOXY-2-(METHOXYCARBONYL)
-3-PENTYLPHENOXY)-2-PENTYL-, METHYL ESTER/CN
E2 1 BENZOIC ACID, 4,6-DIMETHOXY-3-METHYL-2-(1-OXOBUTOXY)-,
METHY
L ESTER/CN
E3 0 --> BENZOIC ACID, 4-(AMINOIMINOMETHYL)AMINO-, 2,2-DIMETHYLPROP
YL ESTER/CN
E4 1 BENZOIC ACID,
4-(((((((2,3-DIHYDRO-2,2-DIMETHYL-7-BENZOFURA

NYL) OXY) CARBONYL) METHYLAMINO) CARBONYL) AMINO) SULFONYL) AMINO) -
 , ETHYL ESTER/CN

E5 1 BENZOIC ACID,
4-((((((2,3,4-TRICHLOROPHENYL) THIO) ACETYL) OXY
) ACETYL) AMINO) METHYL) -, METHYL ESTER/CN

E6 1 BENZOIC ACID,
4-((((((3.BETA.)-17-OXOANDROST-5-EN-3-YL) AMIN
 O) CARBONYL) OXY) METHYL) AMINO) -, 2-(DIETHYLAMINO) ETHYL
ESTER/C

N
E7 1 BENZOIC ACID,
4-((((((3.BETA.)-17-OXOANDROST-5-EN-3-YL) OXY)
 METHYL) THIO) METHYL) AMINO) -, 2-(DIMETHYLAMINO) ETHYL ESTER/CN

E8 1 BENZOIC ACID,
4-((((((3.BETA., 17.BETA.)-3-HYDROXYANDROST-5-
 EN-17-YL) AMINO) CARBONYL) OXY) METHYL) AMINO) -,
2-(DIETHYLAMINO)

ETHYL ESTER/CN
E9 1 BENZOIC ACID,
4-((((((4-BROMO-8-CHLORO-1-NAPHTHALENYL) THIO)
 ACETYL) OXY) ACETYL) AMINO) METHYL) -, METHYL ESTER/CN

E10 1 BENZOIC ACID,
4-((((((4-CHLOROPHENYL) AMINO) CARBONYL) HYDRAZO
 NO) PHENYLMETHYL) THIO) METHYL) -, 1,1-DIMETHYLETHYL ESTER/CN

E11 1 BENZOIC ACID,
4-((((((4-CHLOROPHENYL) SULFONYL) AMINO) PHENYLM
 ETHYLENE) AMINO) THIOXOMETHYL) AMINO) -/CN

E12 1 BENZOIC ACID,
4-((((((4-METHOXYPHENYL) SULFONYL) (PHENYLMETHY
 L) AMINO) ACETYL) AMINO) OXY) DIPHENYLMETHYL) -/CN

=> e Benzoic acid, 4-((aminoiminomethyl) amino) -, 2,2-dimethylpropyl ester/cn

E1 1 BENZOIC ACID, 4-((AMINOIMINOMETHYL) AMINO) -, 1-NAPHTHALENYL
E

STER, METHANESULFONATE/CN
E2 1 BENZOIC ACID, 4-((AMINOIMINOMETHYL) AMINO) -, 1-NAPHTHALENYL
E

STER, MONONITRATE/CN
E3 1 --> BENZOIC ACID, 4-((AMINOIMINOMETHYL) AMINO) -,
2,2-DIMETHYLPROP

YL ESTER/CN
E4 1 BENZOIC ACID, 4-((AMINOIMINOMETHYL) AMINO) -,
2,3-DIFLUOROPHEN

YL ESTER/CN
E5 1 BENZOIC ACID, 4-((AMINOIMINOMETHYL) AMINO) -,
2,3-DIFLUOROPHEN

YL ESTER, MONOACETATE/CN
E6 1 BENZOIC ACID, 4-((AMINOIMINOMETHYL) AMINO) -,
2,3-DIMETHOXYPHE

NYL ESTER, MONOHYDROCHLORIDE/CN
E7 1 BENZOIC ACID, 4-((AMINOIMINOMETHYL) AMINO) -,
2,3-DIMETHYLPHEN

YL ESTER/CN
E8 1 BENZOIC ACID, 4-((AMINOIMINOMETHYL) AMINO) -,
2,3-DIMETHYLPHEN

YL ESTER, MONOMETHANESULFONATE/CN
E9 1 BENZOIC ACID, 4-((AMINOIMINOMETHYL) AMINO) -,
2,4-DINITROPHENY

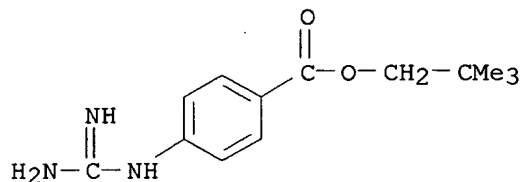
E10 1 L ESTER/CN
 2,5-DICHLOROPHEN BENZOIC ACID, 4-((AMINOIMINOMETHYL)AMINO)-,
 E11 1 YL ESTER/CN
 2,5-DICHLOROPHEN BENZOIC ACID, 4-((AMINOIMINOMETHYL)AMINO)-,
 E12 1 YL ESTER, MONOMETHANESULFONATE/CN
 2,6-DICHLORO-4-N BENZOIC ACID, 4-((AMINOIMINOMETHYL)AMINO)-,
 ITROPHENYL ESTER/CN

=> e3

L15 1 "BENZOIC ACID, 4-((AMINOIMINOMETHYL)AMINO)-,
 2,2-DIMETHYLPROPYL
 ESTER"/CN

=> d 115

L15 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2003 ACS
 RN 282718-30-3 REGISTRY
 CN **Benzoic acid, 4-[(aminoiminomethyl)amino]-, 2,2-dimethylpropyl ester**
 (9CI) (CA INDEX NAME)
 FS 3D CONCORD
 MF C13 H19 N3 O2
 SR CA
 LC STN Files: CA, CAPLUS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1957 TO DATE)
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=> 115

L16 1 L15

=> d 116 ti fbib abs

L16 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2003 ACS

TI (4-aminomethyl)phenylguanidine derivatives as nonpeptidic highly selective

inhibitors of human urokinase

AN 2000:341443 CAPLUS

DN 133:99075

TI (4-aminomethyl)phenylguanidine derivatives as nonpeptidic highly selective

inhibitors of human urokinase

AU Sperl, Stefan; Jacob, Uwe; De Prada, Nuria Arroyo; Sturzebecher, Jorg; Wilhelm, Olaf G.; Bode, Wolfram; Magdolen, Viktor; Huber, Robert;

Moroder,

Luis

CS Max-Planck-Institut fur Biochemie, Martinsried, 82152, Germany

SO Proceedings of the National Academy of Sciences of the United States of America (2000), 97(10), 5113-5118
CODEN: PNASA6; ISSN: 0027-8424

PB National Academy of Sciences

DT Journal

LA English

AB Increased expression of the serine protease urokinase-type plasminogen activator (uPA) in tumor tissues is highly correlated with tumor cell migration, invasion, proliferation, progression, and metastasis. Thus inhibition of uPA activity represents a promising target for antimetastatic therapy. So far, only the x-ray crystal structure of uPA inactivated by H-Glu-Gly-Arg-chloromethylketone has been reported, thus limited data are available for a rational structure-based design of uPA inhibitors. Taking into account the trypsin-like arginine specificity of uPA, (4-aminomethyl)phenylguanidine was selected as a potential P1 residue

and iterative derivatization of its amino group with various hydrophobic residues, and structure-activity relationship-based optimization of the spacer in terms of hydrogen bond acceptor/donor properties led to N-(1-adamantyl)-N'-(4-guanidinobenzyl)urea as a highly selective

nonpeptidic uPA inhibitor. The x-ray crystal structure of the uPA B-chain complexed with this inhibitor revealed a surprising binding mode consisting of the expected insertion of the phenylguanidine moiety into the S1 pocket, but with the adamantyl residue protruding toward the hydrophobic S1' enzyme subsite, thus exposing the ureido group to hydrogen-bonding interactions. Although in this enzyme-bound state the inhibitor is crossing the active site, interactions with the catalytic residues Ser-195 and His-57 are not obsd., but their side chains are spatially displaced for steric reasons. Compared with other trypsin-like serine proteases, the S2 and S3/S4 pockets of uPA are reduced in size because of the 99-insertion loop. Therefore, the peculiar binding mode of the new type of uPA inhibitors offers the possibility of exploiting optimized interactions at the S1'/S2' subsites to further enhance selectivity and potency. Because crystals of the uPA/benzamidine complex allow inhibitor exchange by soaking procedures, the structure-based design of new generations of uPA inhibitors can rely on the assistance of x-ray anal.

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 ENERGY, INSPEC
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